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A General Framework for Regularized Evaluation of Unstable Operators*

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A general approach is developed for stable evaluation of unbounded operators when the data are corrupted by error. The essence of the approach is to recast the direct problem of evaluating the unstable operator as an inverse problem involving an associated bounded operator. Classical general regularization methods for inverse problems are then elucidated within the new setting, and new order optimal parameter choice strategies for iterative and noniterative regularization methods are developed. Finally, a regularizing stopping rule for a conjugate gradient acceleration of Lardy's method is provided.

1. INTRODUCTION

In the past two decades the notion of regularization methods has been developed as a tool to approximate the solution x of an ill-posed *inverse problem*

$$Kx = g,$$

where K is a bounded linear operator which lacks a continuous (generalized) inverse. Integral equations of the first kind can be considered as

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prototype problems of this sort, and there is a variety of applications in the natural sciences which lead to ill-posed inverse problems, cf., e.g., [2, 6].

However, there are also *direct problems*

$$Lx = y, \tag{1.1}$$

where y is to be evaluated, that are ill-posed because L is an unbounded operator; numerical differentiation is a well-known example for this kind of ill-posed problem. Often, regularization methods for a stable evaluation of (1.1) can be derived by recasting the direct problem as an equivalent inverse problem. For example, the problem of numerical differentiation can be rewritten as a first kind integral equation with a Green's function kernel.

For some unbounded operators, however, e.g., for integro-differential operators, such transformations fail because the operator L has nonclosed range. As an example consider the elliptic differential equation

$$-\operatorname{div}(a\nabla u) = f \tag{1.2}$$

in a domain $\Omega \subset \mathbb{R}^n$ with boundary data

$$u = q \qquad \text{on } \partial\Omega. \tag{1.3}$$

Assuming that the conductivity $a \in H^2(\Omega)$ is bounded from below by a positive constant and Ω has sufficiently smooth boundary, problem (1.2), (1.3) has a unique solution $u = F(a) \in H^2(\Omega) \cap H_0^1(\overline{\Omega})$. A typical inverse problem is the determination of the conductivity a from the potential field u. Note that this is a nonlinear problem. A first step in approaching this problem may therefore be linearization. The Fréchet derivative of F is given by

$$F'(a)h = A(a)^{-1}D(a)h,$$

with

$$A(a)w = -\operatorname{div}(a\nabla w) \qquad \text{and} \qquad D(a)h = \operatorname{div}(h\nabla F(a)).$$

Under certain assumptions on a and $F(a)$, the operators $A(a)$ and $D(a)$ are closed injective linear operators on subspaces of $H^2(\Omega)$, resp. $H^1(\Omega)$, with appropriate boundary conditions, cf. Ito and Kunisch [10]. Consequently, the solution of the linearized problem is

$$h = F'(a)^{-1}\tilde{u} = D(a)^{-1}A(a)\tilde{u},$$

i.e., h is given as the solution of a direct problem involving the linear operator $L = D(a)^{-1}A(a)$. Note that the spectrum of L clusters at zero *and* at infinity in general. In other words, L is an unbounded operator with nonclosed range.

A completely different and considerably easier example has been investigated in [7]. The (nonlinear) heat transfer law at the interface of a given solid may be determined numerically by evaluating the integro-differential operator

$$\int_0^t \tilde{\varphi}'(\tau)k(t-\tau)d\tau, \qquad t \geq 0, \tag{1.4}$$

given the measured surface temperature history $\tilde{\varphi}(t)$. Here, the kernal function k in (1.4) depends on the geometry of the problem and, in general, has a mild singularity at the origin. In particular, for a semi-infinite solid the operator

$$(Kx)(t) = \int_0^t x(\tau)k(t-\tau)d\tau$$

is the familiar Abel integral operator, and commutes with the differentiation operator $D\varphi = \varphi'$. In general, however, the operators K and D do not commute, and the spectrum of the operator KD occurring in (1.4) will again cluster at the origin and at infinity.

As a means to regularize direct problems of the form (1.1) given approximate data $\tilde{x}$ Morozov [13] suggested minimizing the quadratic functional

$$\|z - \tilde{x}\|^2 + \alpha\|Lz\|^2 \tag{1.5}$$

over $z \in \mathscr{D}(L)$ for some small $\alpha > 0$. Denoting the minimizer of (1.5) by $\tilde{z}$ he proposed to take $L\tilde{z}$ as approximation of y in (1.1). This approach was subsequently studied in [8] where (among several other results) an a posteriori parameter choice for α has been introduced that provides quasi-optimal approximations Lz of y with respect to the data error in $\tilde{x}$.

In [5] a class of regularization methods for evaluating (1.1) was suggested which parallels the spectral theoretic approach taken earlier for the regularization of inverse problems, cf. e.g., [4, 12, 2]. Although all results in [5, 8] seem to have their natural analog in the context of inverse problems, there has been lacking a rule of how to carry over these results in a general way.

It is the aim of this paper to provide such a rule, and we will demonstrate the potential applicability of this scheme by providing error estimates for the parameter choice rule suggested in [8] for Morozov's

method. Note that no proof for its quasi-optimality was given in [8] because of many tedious technical details.

Another regularization method that fits into the general scheme considered in [5] is the iterative method of Lardy [11] which is defined by a sequence of variational problems. Here, the regularization parameter is the iteration index and the stopping rule thus takes the role of regularization. In the final section we develop some kind of discrepancy principle for stopping the iteration, and again, provide error estimates for the corresponding iterates.

Unfortunately, far too many variational problems have to be solved in a practical implementation of Lardy's scheme. We will therefore describe an accelerated version of this method based on the well-known conjugate gradient method, and again prove the suitability of the discrepancy principle for the termination of this iteration.

Once more it has to be emphasized that all these results have been established earlier in the context of inverse problems, and their extension to direct problems follows comparatively easily from a connection that will be established in the following section.

2. THE BASIC TRANSFORMATION

Let $\mathscr{X}$ and $\mathscr{Y}$ be Hilbert spaces, and L be a closed linear operator

$$L : \mathscr{D}(L) \subset \mathscr{X} \to \mathscr{Y}.$$

It shall be assumed throughout that $\mathscr{D}(L)$ is a dense subset of $\mathscr{X}$, and $\mathscr{R}(L)$ is dense in $\mathscr{Y}$. Following [5] define

$$\check{L} = (I + L^*L)^{-1}, \qquad \hat{L} = (I + LL^*)^{-1}. \tag{2.1}$$

Both operators in (2.1) are bounded and selfadjoint with spectra in $[0, 1]$, cf., e.g., [1].

Assume that we want to determine

$$y = Lx$$

from approximations x^δ of x which are close in the sense that

$$\|x - x^\delta\| \leq \delta \tag{2.2}$$

for some small $\delta > 0$. To this end let $\{T_\alpha : \alpha > 0\}$ be a family of bounded real-valued functions with

$$\begin{aligned} T_\alpha(\lambda) &\to \frac{1}{\lambda}, \qquad \text{pointwise on } (0,1] \text{ as } \alpha \to 0, \\ |\lambda T_\alpha(\lambda)| &\le c, \qquad \text{uniformly for all } \alpha > 0 \text{ and } \lambda \in [0,1]. \end{aligned} \tag{2.3}$$

We define approximations of Lx by choosing

$$x_\alpha^\delta = \check{L} T_\alpha(\check{L}) x^\delta, \qquad y_\alpha^\delta = L x_\alpha^\delta. \tag{2.4}$$

One can think of x_α^δ as being a mollification of the perturbed data x^δ. As shown in [5], x_α^δ belongs to $\mathscr{D}(L)$, and

$$y_\alpha^\delta \to Lx^\delta \qquad \text{if } x^\delta \in \mathscr{D}(L).$$

Otherwise $\|y_\alpha^\delta\| \to \infty$ as $\alpha \to 0$, and a proper choice of $\alpha = \alpha(\delta)$ will provide a *regularized approximation* of Lx.

Instead of the continuous (regularization) parameter $\alpha > 0$ one can also consider approximations indexed by nonnegative integers $n \in \mathbb{N}_0$. In this case we shall speak of *iterative regularization*, and consider the limit $n \to \infty$ rather than $\alpha \to 0$ as above.

Two particular examples from the literature fit into this general scheme. The minimizer x_α^δ (and the corresponding approximation $y_\alpha^\delta = L x_\alpha^\delta$) of (1.5) as suggested by Morozov [13] is obtained for

$$T_\alpha(\lambda) = \frac{1}{\alpha(1-\lambda) + \lambda}. \tag{2.5}$$

Lardy's iterative scheme [11], which will be described in more detail in Section 4, is obtained from the polynomials

$$T_n(\lambda) = \sum_{j=0}^{n-1} (1-\lambda)^j.$$

We will now derive a relation between the above approach of constructing general regularization methods for the evaluation of unbounded operators with the more classical setting concerning the regularization of inverse problems. To this end recall that the selfadjoint positive definite operators $\check{L}$, $\hat{L}$, L^*L, and LL^* all admit arbitrary positive powers, cf., e.g., [1]. Concerning these operators we state the following lemma.

LEMMA 1. *For any real* $\nu > 0$ *we have* $\mathscr{D}((LL^*)^\nu) = \mathscr{R}(\hat{L}^\nu)$ *and* $\mathscr{D}((L^*L)^\nu) = \mathscr{R}(\check{L}^\nu)$.

Proof. For a natural number ν it is obvious that $\mathscr{D}((LL^*)^\nu) = \mathscr{D}((I + LL^*)^\nu)$. Since the latter subset equals $\mathscr{R}(\hat{L}^\nu)$ by the definition (2.1) of $\hat{L}$ the first assertion is obviously fulfilled by $\nu \in \mathbb{N}$. For real ν the claim therefore follows by interpolation, cf., e.g., [1]. The second statement is proved in the same way. ∎

In particular, Lemma 1 implies that $\mathscr{R}(\check{L}^{1/2}) \subset \mathscr{D}(L)$. hence, we can define new (true and perturbed) "data"

$$w = L\check{L}^{1/2}x, \qquad w^\delta = L\check{L}^{1/2}x^\delta. \tag{2.6}$$

The operator $L\check{L}^{1/2}$ has the following properties.

LEMMA 2. $L\check{L}^{1/2} : \mathscr{X} \to \mathscr{Y}$ *is a bounded operator with norm* $\|L\check{L}^{1/2}\| \leq 1$. *Moreover, the following identity holds*:

$$(L\check{L}^{1/2})^*(L\check{L}^{1/2}) = I - \hat{L}. \tag{2.7}$$

Proof. We first recall from [5, Lemma 2.2] that $L\check{L}^{1/2}x = \hat{L}^{1/2}Lx$ for $x \in \mathscr{D}(L)$. Thus, for a fixed $x \in \mathscr{D}(L)$ and any $z \in \mathscr{D}(L)$ we have

$$\begin{aligned}\langle (L\check{L}^{1/2})^*L\check{L}^{1/2}x, z\rangle &= \langle L\check{L}^{1/2}x, L\check{L}^{1/2}z\rangle \\ &= \langle \hat{L}^{1/2}Lx, \hat{L}^{1/2}Lz\rangle = \langle L^*\hat{L}Lx, z\rangle.\end{aligned}$$

Now, obviously,

$$L^*\hat{L}L = L^*L\check{L} = (I + L^*L - I)\check{L} = I - \check{L}$$

on $\mathscr{D}(L)$ showing that

$$\langle (L\check{L}^{1/2})^*L\check{L}^{1/2}x, z\rangle = \langle (I - \check{L})x, z\rangle$$

for all z in the dense subset $\mathscr{D}(L)$ of $\mathscr{X}$. Thus (2.7) has been established for $x \in \mathscr{D}(L)$, and it extends to the whole space $\mathscr{X}$ since $I - \check{L}$ is a bounded operator on $\mathscr{X}$. From (2.7) follows further that

$$\|L\check{L}^{1/2}\|^2 = \|(L\check{L}^{1/2})^*(L\check{L}^{1/2})\| = \|I - \check{L}\| \leq 1,$$

and the proof is complete. ∎

A spectral analysis easily reveals that $\|L\check{L}^{1/2}\| = 1$ if and only if L is an unbounded operator, i.e., if and only if the direct problem (1.1) is ill-posed.

As we will establish below in Proposition 3 the desired quantity $y = Lx$ is a solution of the "*inverse problem*"

$$\hat{L}^{1/2} y = w. \tag{2.8}$$

If L is unbounded then the spectrum of $\hat{L}$ clusters at the origin, and hence, the solution of (2.8) is ill-posed. Concerning the perturbed data w^δ we conclude from Lemma 2 and (2.2) that

$$\|w - w^\delta\| = \|L\check{L}^{1/2}(x - x^\delta)\| \le \|x - x^\delta\| \delta. \tag{2.9}$$

PROPOSITION 3. *Let $w = L\check{L}^{1/2}x$ with $x \in \mathscr{X}$. Then $w \in \mathscr{R}(\hat{L}^{1/2})$ if and only if $x \in \mathscr{D}(L)$. If $x \in \mathscr{D}(L)$ then $y = Lx$ is the unique solution of* (2.8).

Proof. As noted above, if $x \in \mathscr{D}(L)$ then

$$w = L\check{L}^{1/2}x = \hat{L}^{1/2}Lx \in \mathscr{R}(\hat{L}^{1/2}),$$

and $y = Lx$ is a solution of $\hat{L}^{1/2}y = w$. Since $\hat{L}^{1/2}$ is injective this solution is unique. Vice versa, if $w \in \mathscr{R}(\hat{L}^{1/2})$ then $\hat{L}^{1/2}w \in \mathscr{R}(\hat{L})$, which equals $\mathscr{D}(LL^*)$ by Lemma 1. This means that

$$L^*\hat{L}^{1/2}w \in \mathscr{D}(L). \tag{2.10}$$

On the other hand we have

$$L^*\hat{L}^{1/2}w = L^*\hat{L}^{1/2}L\check{L}^{1/2}x = L^*L\check{L}x = (I - \check{L})x = x - \check{L}x,$$

and hence, Lemma 1 and (2.10) imply

$$x = L^*\hat{L}^{1/2}w + \check{L}x \in \mathscr{D}(L).$$

This completes the proof. ∎

The general theory of regularization methods (as developed, for example, in [4, 12]) for the solution of a not necessarily selfadjoint equation (2.8) suggests approximations of the form

$$y_\alpha^\delta = T_\alpha(\hat{L})\hat{L}^{1/2}w^\delta = T_\alpha(\hat{L})\hat{L}^{1/2}L\check{L}^{1/2}x^\delta,$$

where the functions T_α should fulfill precisely the same requirements as above, namely (2.3). In other words, the classical theory applied to the inverse problem (2.8) results in the same class of approximations as the theory developed in [5] for the direct problem, cf. (2.4). Note that the classical smoothness assumptions $y \in \mathscr{R}(\hat{L}^\nu)$ readily translate to the direct setting via Lemma 1.

With these prerequisites it is easy to identify the results in [5, Sect. 3] concerning the regularizing properties of the approximations (2.4) for the direct problem as corollaries of the results on inverse problems as given, e.g., in [4, Chap. 3]. It is only the saturation result [5, Theorem 3.5] concerning Morozov's scheme (1.5) which cannot be obtained in this straightforward manner.

In the following sections we will use this new insight into the approximations (2.4) to obtain some important further results.

3. A POSTERIORI PARAMETER CHOICE RULES

Following Engle and Gfrerer [3], or Raus [14], the best possible worst case error of the regularization method (2.4) for a given function $x \in \mathscr{X}$ is defined as

$$\tilde{\psi}(\delta) := \sup\{\inf\{\|Lx - y_\alpha^\delta\| : \alpha > 0\} : \|x - x^\delta\| \le \delta\}.$$

On the other hand, if $\alpha(\delta)$ denotes a parameter choice strategy depending on the noise level δ in (2.2) then the worst case error of this parameter choice rule is given as

$$\psi(\delta) := \sup\{\|Lx - y_{\alpha(\delta)}^\delta\| : \|x - x^\delta\| \le \delta\}.$$

A parameter choice strategy is called *quasi-optimal* if

$$\psi(\delta) \le c\tilde{\psi}(\delta)$$

for some $c > 0$.

Consider once again Morozov's method (1.5) of computing approximations y_α^δ of Lx. In [8], the following method for choosing the regularization parameter α has been suggested.

Parameter Choice Rule for Morozov's Methods. Choose $\alpha = \alpha(\delta)$ as the solution of the equation

$$\langle x^\delta, \left[\alpha(I - \check{L})T_\alpha(\check{L})\right]^3 x^\delta\rangle^{1/2} = \tau\delta. \tag{3.1}$$

As stated in [8] the nonlinear equation (3.1) has a unique solution, and one could follow the line of argument in [3] to prove the quasi-optimality of this method. Here we will use the results of the foregoing section to prove a slightly weaker result which allows the following error bounds.

THEOREM 4. *Let $x \in \mathscr{D}(L)$, and $\tau > 1$ be fixed. For given data x^δ subject to* (2.2) *determine $\alpha(\delta)$ from* (3.1). *Then $y_{\alpha(\delta)}^\delta \to Lx$ as $\delta \to 0$. Moreover, if*

$x \in \mathscr{D}((LL^*)^\nu L)$ for some $0 < \nu \le 1$ then

$$\|Lx - y^\delta_{\alpha(\delta)}\| = O(\delta^{2\nu/(2\nu+1)}), \qquad \delta \to 0. \tag{3.2}$$

Proof. The functions T_α of (2.5) satisfy Assumptions 2.1 and 2.10 in [3] with

$$g(\alpha) = 1/\alpha, \qquad L = 2, \qquad \tilde{\alpha}(\lambda) = \lambda.$$

Actually these assumptions are only fulfilled for $\lambda \in (0, 1)$ but this causes no problems because $\hat{L}$ has no eigenspace corresponding to $\lambda = 1$ since $\mathscr{R}(\hat{L})$ is a dense subset of $\mathscr{Y}$. Engl and Gfrerer now suggest to choose the regularization parameter $\alpha = \alpha(\delta)$ for the inverse problem (2.8) as the solution of the equation [3, (2.17)], which here takes the particular form

$$\langle w^\delta, 2\alpha^3 (I - \check{L})^2 \big[T_\alpha(\check{L})\big]^3 w^\delta \rangle = \gamma\delta^2, \tag{3.3}$$

where $\gamma \ge L = 2$. Note that the projector Q onto the closure of the range of $\hat{L}$ is the identity operator by virtue of Lemma 1 since $\mathscr{R}(L)$ is assumed to be dense in $\mathscr{Y}$. Using (2.6) and the identity (2.7), we recognize (3.3) as being identical to the parameter choice strategy (3.1). As is shown in [3, Theorem 2.11] this parameter choice strategy is quasi-optimal *with respect to perturbations in w* of order δ.

Although this does not imply quasi-optimality with respect to perturbations in x of order δ, it suffices to conclude the assertions of the theorem. To this end we note first that we have

$$|T_\alpha(\lambda)| \le 1/\alpha, \qquad |\lambda^\nu (1 - \lambda T_\alpha(\lambda))| \le c_\nu \alpha^\nu, \quad 0 < \nu \le 1.$$

From this and [4, Theorem 2.3.3] we conclude that $y^\delta_\alpha \to Lx$ provided

$$\alpha \to 0, \qquad \delta^2/\alpha \to 0.$$

Note that $\|w - w^\delta\| \le \delta$ by virtue of (2.9). On the other hand, if $x \in \mathscr{D}((LL^*)^\nu L)$ for some $0 < \nu \ne 1$ then the choice $\alpha \sim \delta^{1/(2\nu+1)}$ leads to the error estimate (3.2), cf., e.g. [12, Satz 3.4.3]. Now the assertions of the theorem follow from the quasi-optimality of the parameter choice strategy (3.1) with respect to the perturbations in w. ∎

4. LARDY'S METHOD AND CONJUGATE GRADIENTS

Lardy's iteration method, cf. [11], consists in the following procedure: given an initial approximation $x_0 = x_0^\delta \in \mathscr{D}(L)$ of x^δ, compute

$$x^\delta_{n+1} = x^\delta_n + \check{L}\big(x^\delta - x^\delta_n\big), \qquad y^\delta_{n+1} = Lx^\delta_{n+1}, \quad n \in \mathbb{N}_0. \tag{4.1}$$

Recall that the range of $\check{L}$ is contained in $\mathscr{D}(L)$ by Lemma 1, and hence, this iterative scheme is well-defined.

A practical implementation will probably utilize the following weak formulation: given any $x \in \mathscr{X}$, the quantities $z = \check{L}x$ and $y = Lz$ satisfy

$$\langle x, v\rangle + \langle Lx, Lv\rangle = \langle z, v\rangle \qquad \text{for all } v \in \mathscr{D}(L). \tag{4.2}$$

It is obvious from (4.1) that the approximations y_n^δ of Lardy's method are nothing else than the iterates of the classical Landweber iteration applied to (2.8). In this context the discrepancy principle is a useful stopping rule, i.e., parameter choice strategy for $n = n(\delta) \in \mathbb{N}_0$. This requires the evaluation of the so-called discrepancy $\|w^\delta - \hat{L}^{1/2} y_n^\delta\|$, which can be done by virtue of (2.7) as

$$\begin{aligned} \|w^\delta - \hat{L}^{1/2} y_n^\delta\|^2 &= \|L\check{L}^{1/2}\big(x^\delta - x_n^\delta\big)\|^2 \\ &= \langle x^\delta - x_n^\delta, (L\check{L}^{1/2})^*(L\check{L}^{1/2})\big(x^\delta - x_n^\delta\big)\rangle \\ &= \langle x^\delta - x_n^\delta, (I - \check{L})\big(x^\delta - x_n^\delta\big)\rangle. \end{aligned} \tag{4.3}$$

Thus, the discrepancy principle for the Landweber iteration yields the following stopping rule for Lardy's method.

Stopping Rule for Lardy's Method. Choose $n = n(\delta)$ as the smallest nonnegative integer for which

$$\langle x^\delta - x_n^\delta, x^\delta - x_{n+1}^\delta\rangle \le \tau\delta. \tag{4.4}$$

THEOREM 5. *If $\tau > 1$ is fixed and $x \in \mathscr{D}(L)$ then the stopping rule* (4.4) *determines a unique (finite) stopping index $n(\delta)$, and $y_{n(\delta)}^\delta \to Lx$ as $\delta \to 0$. If $x \in \mathscr{D}((LL^*)^\nu L)$ for some $\nu > 0$, and if $\|x - x^\delta\| \le \delta$ then*

$$\|Lx - y_{n(\delta)}^\delta\| = O(\delta^{2\nu/(2\nu+1)}), \qquad \delta \to 0.$$

Proof. It is clear from the definition (4.1) of the iterates that (4.3) coincides with the left-hand side of (4.4). Thus the assertions of the theorem follow immediately from Vainikko's results [15] on the discrepancy principle for the Landweber iteration. ∎

We emphasize that each iteration in Lardy's method requires the solution of a linear equation as in (4.2). As compared to the Landweber iteration for inverse ill-pose problems, Lardy's method should therefore not be considered an explicit but rather an implicit iteration method. In fact, each iteration will require approximately the same amount of work as the solution of Morozov's minimization problem for one particular choice

of α. In other words, Lardy's iteration will only be competitive to Morozov's method if it converges rapidly, which will rarely be the case (similar to the Landweber iteration for inverse problems).

We therefore recommend a combination of Lardy's method with an acceleration scheme of conjugate gradient type, i.e., the use of the much faster conjugate gradient method for solving the normal equations corresponding to (2.8), i.e.,

$$\hat{L}y = \hat{L}^{1/2}w = L\check{L}x. \tag{4.5}$$

We refer to [9] for an extensive treatment of the conjugate gradient method for the regularization of inverse problems. For this particular problem the resulting algorithm (i.e., [9, Algorithm 2.2]) looks as follows:

- Compute $z_0^\delta = \check{L}(x^\delta - x_0^\delta)$ and $r_0^\delta = Lz_0^\delta$ as in (4.2)
- $d = z_0^\delta$ and $s = r_0^\delta$
- for $n = 0, 1, \ldots,$
  - —compute $\check{L}d$ and $\hat{L}s = L\check{L}d$ as in (4.2)
  - —$\alpha = \langle r_n^\delta, r_n^\delta \rangle / \langle s, \hat{L}s \rangle$
  - —$x_{n+1}^\delta = x_n^\delta + \alpha d,$
    $y_{n+1}^\delta = y_n^\delta + \alpha s,$
    $z_{n+1}^\delta = z_n^\delta - \alpha \check{L}d,$
    $r_{n+1}^\delta = r_n^\delta - \alpha \hat{L}s$
  - —$\beta = \|r_{n+1}^\delta\|^2 / \|r_n^\delta\|^2$
  - —$d = z_{k+1}^\delta + \beta d,$
    $s = r_{k+1}^\delta + \beta s$

  end for.

In this algorithm r_n^δ is always the residual $\hat{L}^{1/2}w^\delta - \hat{L}y_n^\delta$ corresponding to (4.5). In addition, the algorithm determines

$$z_n^\delta = \check{L}\left(x^\delta - x_n^\delta\right), \qquad n \in \mathbb{N}_0. \tag{4.6}$$

This can easily be seen by induction. Similarly, besides the usual search direction s the quantity d is updated so as to relate to s via $Ld = s$. This allows the evaluation of the following stopping rule for this method.

Stopping Rule for the Conjugate Gradient Method. Choose $n = n(\delta)$ as the smallest nonnegative integer for which

$$\|x^\delta - x_n^\delta\|^2 - \langle x^\delta - x_n^\delta, z_n \rangle \le (\tau\delta)^2. \tag{4.7}$$

We have the following results for this stopping rule.

THEOREM 6. *If $\tau > 1$ is fixed and $x \in \mathscr{D}(L)$ then the stopping rule* (4.7) *determines a unique* (*finite*) *stopping index $n(\delta)$, and $y_{n(\delta)}^{\delta} \to Lx$ as $\delta \to 0$. If $x \in \mathscr{D}((LL^*)^{\nu}L)$ for some $\nu > 0$, and if $\|x - x^{\delta}\| \le \delta$ then*

$$\|Lx - y_{n(\delta)}^{\delta}\| = O(\delta^{2\nu/(2\nu+1)}), \qquad \delta \to 0. \tag{4.8}$$

Proof. To prove this result we have to show that the left-hand side expression in (4.8) coincides with the square of the discrepancy $\|w^{\delta} - \hat{L}^{1/2} y_n^{\delta}\|$. Comparing (4.7) and (4.3) we observe that this is the case if and only if

$$\langle x^{\delta} - x_n^{\delta}, z_n \rangle = \langle x^{\delta} - x_n^{\delta}, \check{L}(x^{\delta} - x_n^{\delta}) \rangle.$$

Because of (4.6) this is indeed the case. In other words, the stopping rule (4.7) is the usual discrepancy principle for the conjugate gradient method applied to the normal equation of (2.8), and hence, the assertions follow from the analysis of the conjugate gradient method for inverse problems, compare [9, Sect. 3.3]. ∎

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